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Effect of a Periodic Potential on a Degenerate Fermi Gas

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### 1. Introduction

An important problem in understanding the properties of the nuclear surface is the nature of the deviations from the Thomas-Fermi statistical approximation (TFA). According to TFA, the particle and energy density at each point is what it would be if the density were uniform. This approximation is accurate if the density changes sufficiently slowly. However, in the region of the nuclear surface the density & falls from (say) 90% to 10% of its maximum value in a distance comparable with other relevant distances, i.e. the range of nuclear forces and the Fermi wavelength of the system. Thus the effect of inhomogeneity might well be significant here. We assume that the energy density can be expanded in a series of powers of (II) and powers of (7) operating on 3. This is probably a semi-convergent expansion. The odd terms vanish by reflectional invariance of the Hamiltonian. The leading order terms are of the form  $f(f)|f|^2$ +  $\varepsilon(f) p^2 f$ . The latter term can, after partial integration, be cast in the form of the first term; thus only the first will be considered. A correction of this form for the kinetic energy density was first proposed by Weizsäcker<sup>1)</sup>. However, some of his approximations are in error and more recent studies<sup>2)</sup> indicate that the inhomogeneity corrections are much smaller than Weizsäcker gave, although his form

 $f(p) = p^{-1}$ , is preserved.

In this paper we discuss a simple model for generating density variations for which the leading order inhomogeneity effects can be calculated explicity. Instead of trying to study the behavior of particles at the nuclear surface explicitly we consider a set of particles moving independently in a cubical box upon which is superimposed a sinusoidal "ripple" potential.

$$u - \frac{n^2}{2m} a \cos qx \qquad (1)$$

Although this is a different situation than that which exists at the nuclear surface, it is possible to identify uniquely the inhomogeneity correction terms to order  $|\nabla \rho|^2$ . The ripple model has also been considered by Lindhard<sup>3)</sup> in his study of the electron gas.

### 11. CALCULATION OF THE PARTICLE DESIRY

In the absence of the ripple potential, the wave function of each particle is a plane wave:

$$\Phi_{k} = \exp\left[i k \cdot x\right] = \exp\left[i k_{x}x + i k_{y}y + i k_{z}z\right].(2)$$

(We assume periodic boundary conditions and a bost of unit volume). The presence of the ripple potential changes the wavefunction of each particle; however the total wavefunction is still an antisymmetrized product of single particle wavefunctions, as we neglect correlations due to two body interactions. Lince the ripple depends only on the x-coordinate, the y and z-depends t factors are unchanged. However the x-dependent part of each new single particle wavefunction is a Mathieu function. We can, instead, express the new wavefunctions in terms of the original plane waves by a perturbation expansion. Up to second order in the potential the wavefunction corresponding to an imperturbed memoritum k is given as follows:

$$\psi_{\underline{k}} = E^{-\frac{1}{2}} \Phi_{\underline{k}} \left[ 1 - \frac{a}{2} \left( \frac{e^{icx}}{D_{1}(\underline{k})} + \frac{e^{-icx}}{D_{-1}(\underline{k})} \right) + \frac{a^{2}}{4} \left( \frac{e^{2icx}}{D_{1}(\underline{k})D_{2}(\underline{k})} + \frac{e^{-2icx}}{D_{1}(\underline{k})D_{2}(\underline{k})} \right) \right],$$
(3)

where

$$N - 1 + \frac{a^2}{4} \left[ \frac{1}{D_1^2} + \frac{1}{D_1^2} \right]$$

and

$$D_{n}(k) = nq(2k_{x} + nq).$$

The particle density in state k is Liven by:

$$\rho_{k}(x) = \psi_{k}^{*}\psi_{k} = 1 - a\left[\frac{1}{D_{1}} + \frac{1}{D_{-1}}\right] \cos qx + \frac{a^{2}}{2} \left[\frac{1}{D_{1}D_{2}} + \frac{1}{D_{-1}D_{-2}}\right]$$

$$-\frac{1}{D_1D_{-1}}$$
] cos2qx. (4)

To calculate the total particle density, we must sum over all occupied single particle states k. We assume that the particles fill up unperturbed levels in order of increasing energy (neglect any change in level order due to the ripple). Then the number of particles, neglecting spin and isotopic spin, is

$$\sum_{k_{T}^{1}} - A - \sum_{0} - \frac{4\pi}{3} k_{F}^{3}. \tag{5}$$

We also define:

Since the level density is symmetric with respect to the interchange  $k \leftrightarrow -k$  it follows that  $\Phi_{-n} - \Phi$ . The evaluation of the  $a^2$  term can be simplified by use of the identities:

$$\frac{1}{D_1 D_2} - \frac{1}{q^2} \left[ \frac{1}{2D_1} - \frac{1}{D_2} \right], \tag{7a}$$

$$\frac{1}{D_{-1}D_{-2}} = \frac{1}{2q^2} \left[ \frac{1}{D_1} + \frac{1}{D_{-1}} \right]. \tag{7b}$$

Thus we obtain

$$S(x) = \sum_{k} g_{k}(x) - g_{0}(1 - a + a^{2} e^{-2} + a^{2} e^{-2} + a^{2} e^{-2} = e^{-2} =$$

Text we calculate  $\Phi_1$  and  $\Phi_2$ .

In general we have

$$\oint_{n} = P \int_{\frac{Ck}{nc_{x}(2k_{x} + nc_{1})}} \int_{0}^{\infty} dk$$
 (9)

The volume element is dk = 2\pi ki dk dk x

with the region of integration for ky going from o to  $(k_F^2 - k_X^2)^{\frac{1}{2}}$ , and P indicates that singularities are to be treated in the sense of principal value.

Thus be obtain:

$$\oint_{n} = \frac{3P}{4k_{F}^{3}} \qquad \int_{-k_{F}}^{k_{F}} \frac{(k_{F}^{2} - k_{X}^{2})dk_{X}}{nq(2k_{X} + nq)}.$$
(10)

Now introduce new variables:

$$k - k_F \times$$

$$nq = 2k_F y$$
.

l'hen

$$\Phi_{n} - \frac{3}{16k_{F}^{2}} P \int_{-1}^{1} \frac{(1-x^{2})dx}{y(x+y)}.$$
 (11)

A straigthforward calculation gives:

$$\oint_{n} -\frac{3}{16k_{F}^{2}} \left[ 2 + \frac{1-y^{2}}{|y|} \ln \left| \frac{1+y}{1-y} \right| \xrightarrow{\mathbf{q} \to \mathbf{p}} \frac{3}{4k_{F}^{2}} - \frac{n^{2}q^{2}}{16k_{F}^{2}} + \mathcal{O}(q^{4}) \right] (12)$$

In the limit q -> o, corresponding to a long wavelength ripple, the expression for the density becomes

$$g = g_0(1 - \frac{3a}{2k_p^2}) \cos x + \frac{3}{16} \frac{a^2}{k_p^2} \cos 2x$$
 (13)

This agrees, to order a<sup>2</sup>, with the Thomas-Fermi result

$$\mathcal{P}_{TF}(x) = (1 - \frac{3}{16} \frac{a^2}{k_F^2})(1 - \frac{a}{k_F^2} \cos x)^{3/2}$$
 (14)

### III. KINETIC ENERGY

We now turn to the inhomogeneity correction to the kinetic energy. The expectation value of the kinetic energy of a particle in state k is given, in units of  $\hbar^2/2m$ , by

$$T_{k} = -\int \psi_{k}^{*} \int^{2} \psi_{k} d\mathbf{r} - \int \psi_{k}^{*} \nabla \psi_{k} d\mathbf{r}$$
(15)

Substitution of (3) into (15) yields

$$T_{k} = k^{2} + \frac{a^{2}}{4} \left( \frac{1}{D_{1}(k)} + \frac{1}{D_{-1}(k)} \right),$$
 (16)

and the total kinetic energy becomes

$$T - \sum_{k} T_{k} - \left\{ \frac{3}{5} k_{F}^{2} + \frac{1}{2} a^{2} \right\} A \qquad (17.a)$$

$$\xrightarrow{q \to 0} \left\{ \frac{3}{5} k_F^2 + \frac{3}{8} \frac{a^2}{k_F^2} - \frac{a^2 q^2}{32 k_F^4} \right\} A. \tag{17.b}$$

This result agrees to order a<sup>2</sup> and in the limit q=o with the Thomas-Fermi approximation, according to which

$$T_{TF} = \frac{3}{5}k_{F}^{2} \land \langle (1 + \frac{1}{3}c)^{5/3} \rangle$$

$$= \frac{3}{5}k_{F}^{2} \land [1 + \frac{5}{3}c] \land \frac{3}{9}c \rangle + \frac{5}{9}c (\frac{3}{9}c)^{2} + \dots ], \qquad (18)$$

where < > denotes average over space. According to (13),

$$\frac{\delta e}{S^{\circ}} = -\frac{3a}{2k_{\mathrm{F}}^2} \quad \cos qx + \dots \tag{19}$$

Thus  $\langle \delta p \rangle$  vanishes, but  $\langle (\delta p)^2 \rangle$  is finite. This gives

$$T_{TF} - \frac{3}{5}k_F^2A(1 + \frac{5}{8} + \frac{a^2}{k_F^4} + ...),$$
 (20)

in agreement with (17b).

In a non-unique way, it is possible to discuss the kinetic energy density,  $\tau_k$ , defined by the requirement  $\tau_k = \int \tau_k dr$ . In addition to the forms suggested by Eq.(15), one which is also useful in the calculation of the exchange potential energy is

$$\tau_{\underline{k}}(x) = \frac{1}{4} \left[ -\psi_{\underline{k}}^* (\nabla^2 \psi_{\underline{k}}) + 2(\underline{\nabla} \psi_{\underline{k}}^*) \cdot (\underline{\nabla} \psi_{\underline{k}}) - (\underline{\nabla}^2 \psi_{\underline{k}}^*) \psi_{\underline{k}} \right]$$
(21)

Substitution of the expression for the wavefunction (3) into this definition leads to

$$\mathcal{T}_{\mathbf{x}}^{(\mathbf{x})} = k_{\mathbf{x}}^{2} + \frac{\mathbf{a}^{2}}{4} \left( \frac{(k_{\mathbf{x}} + \mathbf{q})^{2} - k_{\mathbf{x}}^{2}}{D_{1}^{2}} + \left[ \frac{(k_{\mathbf{x}} - \mathbf{q})^{2} - k_{\mathbf{x}}}{D_{-1}^{2}} \right] - \frac{(k_{\mathbf{x}} + \frac{\mathbf{q}}{2})^{2}}{D_{1}} + \frac{(k_{\mathbf{x}} - \frac{\mathbf{q}}{2})^{2}}{D_{-1}} \right] = \frac{(k_{\mathbf{x}} + \frac{\mathbf{q}}{2})^{2}}{D_{1}D_{2}} + \frac{(k_{\mathbf{x}} - \mathbf{q})^{2}}{D_{-1}D_{-2}} + \frac{k_{\mathbf{x}}^{2}}{D_{1}D_{-1}} \right] = \frac{\mathbf{a}^{2}}{4} \cos 2q\mathbf{x} + (k_{\mathbf{y}}^{2} + k_{\mathbf{z}}^{2}) + \frac{\mathbf{k}^{2}}{2} + \frac$$

By means of some elementary algebraic manipulation we can simplify this formula to

Summing over states k, we obtain

where here  $\langle \rangle$  denotes average over the distribution. The total kinetic energy is the spatial integral of (24), which gives Eq.(17).\*

\* Although the average kinetic energy density is given correctly by TFA, the explicit impression is not quite correct. According to TFA, the kinetic energy density should be isotropic at each point. On the other hand, according to our ripple model, the y-component of the kinetic energy density is given by

$$g < k_y^2 > -\frac{1}{5}k_F^2 g$$

while the x component is not simply proportional to the density. This discrepancy may be connected with the fact that we have not taken into account rearrangement of the level order due to the ripple potential; i.e. the levels are assumed to fill up in order of increasing unperturbed energy, which may not necessarily imply order of increasing perturbed energy.

In order to interpret the nature of the  $q^2$  terms, we reconsider the expression for  $\delta \rho$ :

$$\frac{\delta P}{P \circ} = -\frac{2a}{3k_F^2} \left(1 - \frac{c^2}{12k_F^2}\right) \cos(qx). \tag{25}$$

Clearly

It can be readily verified that the change in kinetic energy due to the ripple equals

$$\delta T = \frac{\frac{12}{2}}{\frac{2}{3}} \langle (\delta S)^2 \rangle + \frac{1}{\frac{2}{3}} \langle |\nabla S|^2 \rangle. \tag{27}$$

The first term is just the correction discussed above, while the second term is an inhomogeneity term. This correction can be expressed as

$$\delta T = \frac{\xi}{4} + \frac{|\xi p|^2}{P_0} \tag{28}$$

with

$$\xi - \frac{1}{Q}$$
.

The Weizsäcker correction 1) is of just this form, but with

\( \) = 1. Thus our correction is only 1/9 as large as that calculated by \( \) \( \

It is also of interest to consider the other limit of a rapiuly varying potential, i.e.  $q \gg k_T$ .

In this case we have

and thus

$$\delta T = \frac{a^2}{2a^2} . \tag{30}$$

But in this case

$$\delta g = -\frac{2a \cos qx}{q^2} \tag{31}$$

so that

$$\sum_{c} - \frac{2a \operatorname{singx}}{c} \hat{R}_{x} . \tag{32}$$

Thus we find

$$\delta \tau - \frac{1}{4S_{\circ}} \sqrt{|S|^2}, \qquad (33)$$

which is the same as the Meizsacker correction ( $\xi = 1$ ). However, Weizsäcker's original derivat on was intended to be valid in the limit  $q \rightarrow 0$ .

### IV. INHOMOGENEITY COLLECTIONS TO THE POTESTIAL ENERGY

### we calculate

In this section/inhomogeneity corrections to the potential energy due to a short range two body interaction, but neglect all correlations due to these interactions.

First, consider a local (Wigner) interaction and neglect exchange terms.

The total interaction energy is given by

$$PE^{W} = \frac{1}{2} \sum_{m} \sum_{n} \psi_{m}^{*}(\mathbf{r}_{1}) \psi_{n}^{*} (\mathbf{r}_{2}) V(\mathbf{r}_{1} - \mathbf{r}_{2}) \psi_{m}(\mathbf{r}_{1}) \psi_{n}(\mathbf{r}_{2}) d\mathbf{r}_{1} d\mathbf{r}_{2}, \qquad (34)$$

which equals

$$\frac{1}{2} \iiint g(\mathbf{r}_1) g(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 . \tag{35}$$

Introducing center-of-mass and relative coordinates k, r, we can write this as

$$PE^{W} = \frac{1}{2} \iint P\left(R + \frac{r}{2}\right) P\left(R - \frac{r}{2}\right) V(r) dRdr. \qquad (36)$$

Making a Taylor expansion of the density about its value at R, we find

$$\int_{\mathbb{R}} \frac{(R + \frac{r}{2})}{(R + \frac{r}{2})} \frac{(R - \frac{r}{2})}{(R + \frac{r}{2})} = \int_{\mathbb{R}}^{2} \frac{(R)}{(R)} + \sum_{i} \sum_{j} \frac{1}{4} x_{i} x_{j} \left( \int_{\mathbb{R}} \frac{\partial^{2} f}{\partial x_{i} \partial x_{j}} - \frac{\partial f}{\partial x_{i} \partial x_{j}} - \frac{\partial f}{\partial x_{i} \partial x_{j}} - \frac{\partial f}{\partial x_{i} \partial x_{j}} + \dots \right) (37)$$

To calculate the potential energy, we assume that V is spherically symmetric. Then with help of an integration by parts, we obtain

$$TE^{W} = \frac{1}{2} \int \rho^{2} dR \int V dr - \frac{1}{12} \int |\nabla \rho|^{2} dR \int V r^{2} dr + \Theta(v r^{4} dr).$$
 (38)

The first term represents the potential energy due to a 8-function interaction. The second term is the lowest order classical inhomogeneity term due to the finite range of the nuclear forces.

exchange (Majorana) interaction. This gives

$$PE^{M} = \frac{1}{2} \sum_{m} \sum_{n} \psi_{m}^{*}(\mathbf{r}_{1}) \psi_{n}^{*}(\mathbf{r}_{2}) U(\mathbf{r}_{1} - \mathbf{r}_{2}) \psi_{m}(\mathbf{r}_{2}) \psi_{n}(\mathbf{r}_{1}) d\mathbf{r}_{1} d\mathbf{r}_{2}$$

$$= \frac{1}{2} \iiint \rho^{2}(\mathbf{r}_{1}, \mathbf{r}_{2}) U(\mathbf{r}_{1} - \mathbf{r}_{2}) d\mathbf{r}_{1} d\mathbf{r}_{2}, \qquad (39)$$

where the mixed density  $\rho(r_1,r_2)$  is defined by

$$g(r_1, r_2) = \sum_{m} \psi_{m}^*(r_1) \psi_{m}(r_2). \tag{40}$$

Again, in terms of a center of mass and relative coordinates we obtain

$$PE^{M} = \frac{1}{2} \iiint_{2}^{2} (R + \frac{r}{2}, R - \frac{r}{2}) U(r) divdr.$$
 (41)

Now a simple expansion about R shows that

$$S^{(R+\frac{r}{2}, R-\frac{r}{2})} - S^{(R,R)} - \frac{1}{2} \sum_{i} \sum_{j} x_{i} x_{j} T^{ij},$$
 (42)

where

$$T^{ij(x)} = \frac{1}{4} \sum_{k} \psi_{k}^{*} \frac{\partial^{2} \psi_{k}}{\partial x_{i} \partial x_{j}} + 2 \frac{\partial \psi_{k}^{*} \partial \psi_{k}}{\partial x_{i} \partial x_{j}} - \frac{\partial^{2} \psi_{k}^{*}}{\partial x_{i} \partial x_{j}} \psi_{k} (43)$$

The quantity  $T^{ij}$  is closely related to the kinetic energy density defined in Eq.(24); in fact,

$$\tau(x) - \xi_i \tau^{ii}(x). \tag{44}$$

Thus, for a central potential we obtain

$$PE^{M} = \frac{1}{2} \int g^{2} dR \int U dr - \frac{1}{6} \int g \nabla dR \int U r^{2} dr + \Theta \left( \int U r^{4} dr \right). \tag{45}$$

The volume integral of g can be calculated using (8) and (24). It is seen that the  $q^2$  correction to g is 290 times as large as the correction to T. Thus, the inhomogeneity correction to T equals  $\frac{1}{18} |D_{g}|^{2}$ , and the correction to the exchange potential energy is only 1/9 as large as for a direct potential of the same strength and range \*.

<sup>\*</sup> An exchange interaction appears in this respect like a velocity dependent b-function interaction, for which there is no inhomogeneity correction.

This conclusion appears plausible when e realize that the matrix elements of an exchange interaction depend on the <u>average</u> relative momentum of the colliding pair before and after the scattering but, (like a 8-function), are independent of the momentum transfer in the collision. By contrast, the matrix elements of a finite range <u>local</u> interaction depend only on the momentum <u>transfer</u>, but not on the momenta themselves

### V. ONE AND TWO DIMENSIONAL FERMI GAS

It is possible to obtain additional insight into the nature of the inhomogeneity terms by considering the one and two dimensional analogues of the model considered above. The expressions (8) and (17.a) still hold for the particle and kinetic energy densities. However, the functions  $\Phi$  are now given by different expressions, since the integral over the available phase space is different.

In the one dimensional case, we have

$$\oint_{1} - P \int_{-k_{F}}^{k_{F}} \frac{dk_{x}}{(k_{x}+q)^{2} - k_{x}^{2}} \int_{-k_{F}}^{k_{F}} dk_{x} = \frac{1}{2k_{F}q} P \int_{-k_{F}}^{k_{F}} \frac{dk_{x}}{2k_{x}+q} . \quad (46)$$

Making the same change of variables as in the three dimensional case, we find

An elementary calculation shows that in this case the inhomogeneity sign term has the opposite as the Weizsacker correction and is 1/3 as large i.e. it is given by (28) with  $\frac{1}{3} = -\frac{1}{3}$ . However, if  $q \gg 2k_F$ , then we get exactly the Weizsäcker term, the same as in the three dimensional case.

In the two dimensional case, we have

$$-\left\{\frac{\frac{1}{2k_{F}^{2}}, \quad \text{for } q < 2k_{F}, \\ \frac{1}{2k_{F}^{2}}\left[1 - \left(1 - \frac{4k_{F}^{2}}{q^{2}}\right)^{\frac{1}{2}}\right], \quad \text{for } q > 2k_{F}. \right\}$$
(48)

It is dignificiant that in the two dimensional case, we obtain no inhomogeneity correction ( $\frac{1}{2}$  +  $\frac{1}{2}$ ) for  $\frac{1}{2}$   $\frac{2}{2}$  $\frac{1}{2}$ 

In particular, we find, for  $g \le 2k_F$ ,

$$\int -\int_0^{\pi} \left[1 - \frac{a}{k_F^2} \cos \alpha x\right] \tag{49}$$

with no term of order a<sup>2</sup>,

and

$$T - S_0 \left[ \frac{1}{2} k_F^2 - \frac{3a}{4} \cos \alpha x + \frac{a^2}{4k_F^2} (1 + \frac{1}{2} \cos 2\alpha x) \right].$$
 (50)

The total kinetic energy is

$$T = A \left(\frac{k_F^2}{2} + \frac{a^2}{4k_F^2}\right), \tag{51}$$

which agrees with the exact TFA value.

It is also interesting to note that in the two dimensional case, the density is proportional to the maximum kinetic energy. This linearily is probably closely connected with the absence of the inhomogeneity term.

We would now like to investigate whether there are any corrections to the average kinetic energy involving higher powers of the strength a of the ripple potential. To answer this question, we must calculate higher order corrections to our single particle wavefunctions. It can be demonstrated explicitly that there are no further corrections to the kinetic energy through order a provided  $q \leqslant k_p$ , but we have not verified that Eq.(51) is exact for two dimensions  $(q \le 2k_p)$ . It appears (although not proven) that corrections of order a vanish identically provided  $q \leqslant \frac{2k_p}{n}$ .

### V1. NUCLEAR SURFACE

If the form of the inhomogeneity correction is assumed to be of the form (28) in nuclei, then an analysis<sup>5)</sup> shows that the empirical value of , including both kinetic and potential effects, lies in the range 0.38 to 0.72, depending upon which semi-empirial mass formula is used. Since the kinetic contribution is only 1/9, the remainder must be attributed to potential energy. The results of Section IV show that the contribution to the inhomogeneity of an exchange potential is only 1/9 that of an identical Wigner potential. Since the Wigner and Majorana components of the internucleonic potential appear to be comparable, the major part of the inhomogeneity appears to be derivable from the Wigner part of the potential, i.e., it is a classical rather than a specifically quantum mechanical effect.

While inhomogeneity term is responsible for the finite surface, it contributes just half (exactly half if form (28) is assumed) of the surface energy, the remaining being derived from the loss of binding energy in the surface region as would be computed from (say) a Fermi gas model.

Of course the factor 1/9 is valid only if the effective wavelength of the density variation at the nuclear surface is long compared with the Fermi wavelength, that is,  $q/2k_F \ll 1$ . If this

we estimate this ratio as follows:

We approximate the density on the surface region by  $f = \frac{1}{2} \int_0^\infty \left[1 - \sin qx\right]$ . The 90% to 10% fall off distance D is related to q by qD = 1.86, thus for D = 2.4f and  $k_p = 1.4f^{-1}$ , we find  $q/2k_p = 0.28$ , which appears to be sufficiently small for our purposes.

In conclusion, we reiterate that the analysis is made for an independent particle model with local (including exchange) interactions. A more complete analysis must include the effect of inter-nucleonic correlations.

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# EFFECTS OF A PERIODIC POTENTIAL ON A DECENERATE FERMI GAS

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ABSTRACT: The effect of a periodic potential on the particle and energy density of a degenerate Fermi gas is considered. For a weak and long wavelength potential, the inhowegeneity correction and kinetic energy density is only 1/9 as large as the Weizsacker estimate. The inhomogeneity corrections due to Majorna exchange two-body interactions of short range are only 1/9 as large as for a short range Uigner interaction.